4-Nitrocinnamaldehyde

Other names: p-Nitrocinnamaldehyde
2-Propenal, 3-(4-nitrophenyl)-
Cinnamaldehyde, p-nitro-
Inchi: InChI=1S/C9H7NO3/c11-7-1-2-8-3-5-9(6-4-8)10(12)13/h1-7H/b2-1+
InchiKey: ALGQVMMYDWQDEC-OWOJBTEDSA-N
Formula: C9H7NO3
SMILES: O=CC=Cc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 177.16
CAS: 1734-79-8

Physical Properties

Property code	Value	Unit	Source
gf	143.93	kJ/mol	Joback Method
hf	16.85	kJ/mol	Joback Method
hfus	26.57	kJ/mol	Joback Method
hvap	61.84	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	1.807		Crippen Method
mcvol	128.600	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
tb	641.64	K	Joback Method
tc	893.15	K	Joback Method
tf	410.66	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.05	J/mol×K	641.64	Joback Method
cpg	312.60	J/mol×K	683.56	Joback Method
cpg	322.26	J/mol×K	725.48	Joback Method
cpg	331.10	J/mol×K	767.40	Joback Method
cpg	339.19	J/mol×K	809.32	Joback Method
cpg	346.60	J/mol×K	851.23	Joback Method

cpg	353.41	J/mol×K	893.15	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1734798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume